Topological excitations and second order transitions in 3D $O(N)$ models

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I discuss several examples of critical phenomena in $O(N)$ models where topological excitations play an important role at criticality. I focus particular attention on the $O(2)$ model in 3D, where recent measurements of the vortex string length distribution in equilibrium suggest the existence of a quantitative picture of the critical behavior in terms of defects. The compatibility of this perspective with renormalization group predictions is examined.

1 Overview

Second order phase transitions are the class of critical phenomena best understood theoretically, both through analytical methods and via large scale computational studies. The superb agreement among experiment, the renormalization group predictions and lattice studies for the values of universal critical exponents [1] is one of the major achievements of modern physics.

Most of the models used to describe continuous critical phenomena have interesting topology in two and three spatial dimensions, where they are relevant experimentally. As a result configurations that carry quantized topological numbers are part of their excitation spectrum, together with the more usual low lying hydrodynamic modes.

The understanding of the role of topological and hydrodynamic excitations in these models gives us the best hints about the mechanisms by which long range order, present at low temperatures, is destroyed above some critical $T = T_c$, since, for continuous transitions, the state of (dis)order is reached gradually, from small towards large spatial scales.

In this respect hydrodynamic modes are typically inefficient. The presence of topological excitations, (domain walls, vortices, hedgehogs, textures), by contrast, implies disorder of phases or flows at least locally. Moreover topological excitations can arrange themselves into finite energy configurations. These become likely as a statistical fluctuation above a temperature T comparable with their energy. The size of such configurations is also the spatial extent to which disorder can exist in a macroscopically ordered state.

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In this lecture I will discuss how topological excitations are associated with order-disorder transitions in scalar $O(N)$ models. These models describe critical phenomena in many relevant materials. Examples are liquid-vapor transitions, Ising magnets, the superfluid transition in ^{4}He, transitions in high T_c superconductors and ferromagnets, to name only some of the most familiar.

The importance of a detailed understanding of topological excitations in these materials is far from purely academic. Vortices, for example, promote dissipation in superfluids and superconductors. Controlling them is a an essential step towards rendering these materials amenable to important applications. In addition several recent experiments [2,3,4,5,6] have measured topological defect formation in condensed matter systems with the objective of learning lessons to be extrapolated to similar phenomena in the early Universe.

The outline of this lecture is as follows. In section 2 I discuss two canonical examples: The Ising model and the Kosterlitz-Thouless transition in 2 spatial dimensions (2D). These will illustrate the connection between the spatial occurrence and distributions of topological excitations and the development of long range disorder as T_c is reached from below. I will proceed in section 3 to new results in 3D, which allow us to characterize the transitions exclusively in terms of topological excitations (vortex strings) in $O(2)$. Some conclusions and outlook for the future of research in the field are provided in section 4.

2 Canonical Examples

There are several canonical examples illustrating the connection between topological excitations and the onset of long range disorder that marks critical behavior. Here I will discuss two 2D examples: the Ising ($N = 1$) and the $O(2)$ models, which display complementary features that will later generalize to the more interesting 3D cases. These two examples establish how the thermal occurrence and distributions of point-like and extended topological excitations may lead to eventual long range disorder.

The (nearest neighbor) Ising model in 2D is a thoroughly understood system. On a square lattice the model is exactly solvable. It has a second order phase transition, below which spontaneous macroscopic magnetization appears in the system[b]. The Hamiltonian for the Ising model can be written as

$$H = J \sum_{\langle ij \rangle} (1 - S_i . S_j) \, , \tag{1}$$

where S_i is the spin at point i, $S_i = \pm 1$ and the sum is over nearest neighbors.

[b] This model is in the same universality class as a real $\lambda\phi^4$ field theory. All comments made about critical behavior in the Ising model apply there too.

At low T then there is long range magnetic order, *i.e.*, the spins all point in the same direction, with exceptions limited to very small spatial extents. As T is increased however the thermal state of the system is characterized by ever increasing islands of spins opposite to those of the main cluster, see Fig. 1. At $T = T_c$ these domains become as large as the volume and the magnetization vanishes. At $T > T_c$ the system is disordered and there is no net magnetization, *i.e.* both directions of spin are equally likely.

In the Ising model there is an exact mapping between two kinds of degrees of freedom - the spins and domain walls. Domain walls are sites where the spin changes orientation. Knowing the location of domain walls is completely equivalent to knowing the spins, but contains of course no extra information. A wall has a certain tension σ - its energy per unit length - clearly $\sigma = 2J$.

A different perspective then is that as T is increased walls become larger and at $T = T_c$ they percolate the volume. We can in principle then write the partition function for the Ising model in terms of walls. Since walls are lines in 2D the partition function is that of an ensemble of walks. Assuming periodic boundary conditions further implies that all walks are closed.

Let us try to build the simplest statistical theory of walks. The simplest ensemble of walks is one in which the walks are free, *i.e.*, that being at any point in space they can proceed to any of its nearest neighbors (say on a lattice). Then the partition function is

$$\mathcal{Z} = \mathcal{N} \int DE \; \Omega(E) \; e^{-\beta E}. \tag{2}$$

The energy of the wall is, as we have seen, simply proportional to its length $E = 2Jl/a$,where a is the lattice spacing. The number of configurations $\Omega(E)$ for a walk of length l/a is:

$$\Omega(E) = N^2 z^{l/a} (l/a)^{-2}, \tag{3}$$

where N^2 accounts for all the possible starting points on a $N \times N$ lattice, z is the number of available points at each step, and there are two factors of $(l/a)^{-1}$ one accounting for the probability of a walk to return to the origin after l/a steps (this form is valid for l/a large) and another to remove overcounting since any point on the walk could have been a starting point. We obtain

$$\mathcal{Z} = \mathcal{N} \int Dl \; n(l), \qquad n(l) = (l/a)^{-2} \exp\left[-\beta \sigma_{\text{eff}}(T) l/a\right] \tag{4}$$

with $\sigma_{\text{eff}} = 2J - T\ln(z)$. There is clearly a transition at $T_c = 2J/\ln(z)$. If walks were free in a 2D square lattice $z = 4$, but it is easy to see that to

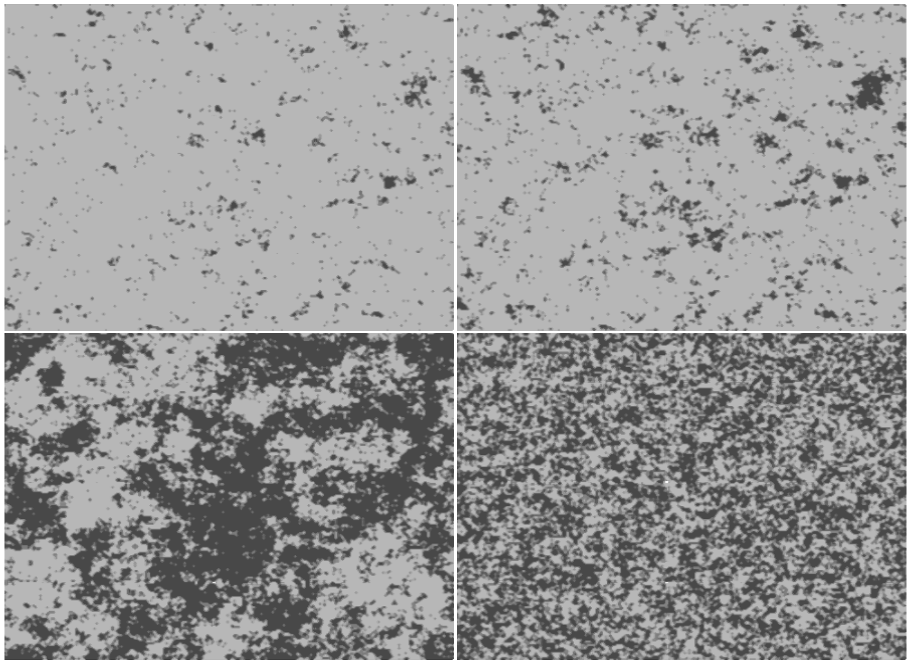

Figure 1: Typical configurations of a 2D Ising model in thermal equilibrium. T increases from left to right and top to bottom, showing how domains of the subdominant phase (black) grow to percolate the volume at $T = Tc$, 1c. At $T > T_c$, 1d, both phases are equally likely but spatial coherence is retained over a length $\xi(T)$.

represent interfaces of spins a walk cannot take a step back so that $z = 3$. This is an excellent approximation to the exact T_c which is $T_c = 2J/\ln(2.639)$. The discrepancy between the exact T_c and our simple model results from the large l/a approximation made in $\Omega(E)$. For some configurations there are in fact only two possible choices in order for the walk not to close after a few steps (e.g. a walk around a single plaquette).

With this example we have seen that the phase transition could be described equally well in terms of domain walls or in terms of more elementary individual spins. The two descriptions are completely equivalent and contain exactly the same information about the system's configuration. Choosing between them is merely a matter of computational convenience.

Our next example is the celebrated Kosterlitz-Thouless transition [7]. This transition occurs in several 2D systems, most notably in ^{4}He films [8]. The transition is usually described in the context of the $O(2)$ (or x-y) model in 2D.

The Hamiltonian is similar in form to (1), but the spins now take values on the circle $S_i = (\cos\theta, \sin\theta)$, $\theta \in \{0, 2\pi\}$, and θ is the phase of the spin. This model is in the same universality class as a *complex* $\lambda\phi^4$ model.

Although the preferred state of the system at low T would seemingly be one with all spins aligned, it turns out that the 2D case, for all $T \neq 0$, is special. Indeed if one had true long range order one would expect that the spin-spin correlator as a function of distance to be:

$$\langle \delta S(x).\delta S(y)\rangle \propto \exp\left[-|x-y|/\xi(T)\right], \tag{5}$$

describing small disturbances δS with a characteristic length ξ, over of a condensate $\langle S\rangle^2 = 1$. Instead in 2D, at low T, one has

$$\langle S(x).S(y)\rangle \sim 1/|x-y|^{\eta(T)}, \tag{6}$$

where the exponent $\eta(T) = T/(2\pi\rho(T))$ is T dependent. This form of the correlation function is typical of a system undergoing a second order transition at criticality, when $\xi \to \infty$. In this sense the behavior of the system at low T is a sequence of critical points characterized by different values of $\eta(T)$.

Nevertheless the system is known to have a transition at high T to a truly disordered state. This transition is due to vortex excitations. How does a vortex induce disorder ? A vortex is a spin configuration where along a closed path in space the phase of the field or spin θ changes by a multiple of 2π. This number is then a quantized topological charge Q

$$Q = \int_\Gamma dl.\vec{\nabla}\theta, \tag{7}$$

where Γ is a closed path in space. If a vortex with winding number N exists within Γ then $Q = 2\pi N$. Vortices can be of either sign and a vortex anti-vortex configuration is topologically trivial.

Because the spins wind around the center of the vortex the phase is disoriented arbitrarily far from the singularity. The presence of this angular phase gradient makes each isolated vortex have infinite energy in the infinite volume limit. The energy divergence as is well known $E = \pi\rho\ln(L/a)$, where L is the linear dimension of the container and the energy ρ is dependent on details of the model. Thus a single vortex configurations cannot occur in a large volume.

The most likely configuration involving vortices is then a pair of vortex-antivortex. If the pair has a separation R it costs an energy $E_{pair} \sim \pi\rho\ln(R/a)$, and introduces phase disorder over a length of order R. Since we must have R small to keep the fluctuation probable this does not seem an efficient way of creating *long-range* disorder. Long range disorder, nevertheless, can come about if we are able to create vortex pairs of arbitrary separations or/and if we can produce enough pairs that the phase is disoriented everywhere, *i.e.* the separation between two pairs is comparable to the pair size.

To dictate which of these mechanisms is relevant we have to understand the thermodynamics of vortices better. If we assume, for a first rough picture, that each new vortex pair does not interact with those already present in the configuration then the number of configurations, with the same energy, is $\Omega(R) = N^2 2\pi R$. The first factor counts all the places on the lattice where we can place the first vortex. The remaining accounts for all positions in 2D, at the distance R, from the first vortex where we can place the second. Thus the entropy of the pair is $S(R) = \ln \Omega(R)$. The free energy of the pair then is

$$F(R) = E(R) - TS(R) \simeq (\pi\rho - T)\ln(R/a). \tag{8}$$

Thus from this simple argument we see that there is a temperature $T_{KT} = \pi\rho$ at which vortices of *any* separation can be created, implying the onset of long range disorder. This simple picture of the transition is qualitatively correct. However to obtain T_c accurately we must account for the fact that ρ *is* changed by the presence of vortices and must therefore be self-consistently determined. This is done via well known Kosterlitz-Thouless relations[9] that yield $\rho(T_{KT})/T_{KT} = 2/\pi$, which is a universal number, confirmed by experiment[8].

Above T_{KT} we must have long range disorder, and the system can be characterized by a correlation length ξ, which is a function of the free-vortex density. The static vortex interaction potential coincides with that for unscreened point charges in 2D. Then, the vortex ensemble can be studied via the Coulomb gas partition function. But once we adopt the Coulomb gas version of the critical phenomenon we have lost contact with our original degrees of freedom - the spins. We have in this way simplified our view of the transition and expressed it in terms of its essential degrees of freedom - the vortices.

The Coulomb gas perspective of the transition in the 2D x-y model supplies us with a new paradigm for the description of phase transitions in terms of topological excitations: that of a transition between a conductor and an insulator. Below the transition there are no *free* vortices, since all appear in pairs of small separation. Thus the charged medium is made out of dipoles and is polarizable but not conducting. At high temperatures some of the charges (vortices) are free and the medium becomes a conductor.

This picture of the behavior of the topological charges as T_{KT} is crossed will prove useful in the step to 3D, where second order transitions with diverging characteristic lengths are the norm.

3 The 3D $O(2)$ model

In 3D $O(N)$ models display second order phase transitions. Of these perhaps the most important is that in the $O(2)$ (or x-y) model. This transition describes critical phenomena in ^{4}He, in extreme type II superconductors [11], and is a canonical model for some of the simplest phase transitions in the early Universe, such as the Peccei-Quinn transition [12].

The role of vortex lines in this model has an illustrious history. Onsager [13] and later Feynman [14] suggested that the phase transition in ^{4}He could be brought about by the proliferation of vortex lines in the superfluid.

The advent of the renormalization group, however, allowed one to solve for the critical behavior of the $O(2)$ model without any reference to vortex configurations at all. The renormalization group results for critical exponents agree with experiment to better than three decimal places. No quantitative picture of the transition based on vortices can rival such feat.

Nevertheless vortex lines exist in the excitation spectrum of the theory. It turns out that one can actually study their behavior by sampling the $O(2)$ partition function. This allows us to generate field configuration characteristic of the thermal state at any given T and search for vortex strings. In this manner we measure the statistical behavior of vortex strings as a function of T. As we discussed above the string population can be fully characterized by the probability distribution function of number of strings *vs.* length.

Free strings, in analogy to domain walls in 2D, are characterized by a length distribution

$$n(l) = Al^{-\gamma} \exp[-\beta\sigma_{\rm eff} l] \tag{9}$$

where $\gamma = 5/2$ and $\sigma = \sigma_{\rm eff} - T\ln(z)$. In general vortex strings are interacting, leading to different values of γ and a different T dependence of $\sigma_{\rm eff}$. The actual value of these parameters as a function of T are shown in Fig 2.

Fig. 2 gives a characterization of the phase transition in terms of vortex strings [17]. Fig. 2a (top left) shows how the total densities of long string $\rho_{\rm inf}$, short loops $\rho_{\rm loop}$ and the total $\rho_{\rm tot}$ change with $\beta = 1/T$. Clearly strings are suppressed below T_c (which was measured independently over field correlators), and long strings appear at $T = T_c$. Fig.2b (top right) shows $n(l)$. Below T_c long strings are exponentially suppressed, while above T_c $n(l)$ becomes scale invariant. The parameters γ and $\sigma_{\rm eff}(T)$ characterizing $n(l)$ are shown in Fig. 2c and finally Fig. 2d (bottom right) shows the exponent γ_l characterizing the scale invariant distribution of long strings ($\gamma_l = 1$ for free long strings in a domain with periodic boundary conditions). Fig. 2d also shows $R(l)$ the distance between two points on the string *vs.* its length. Small string loops

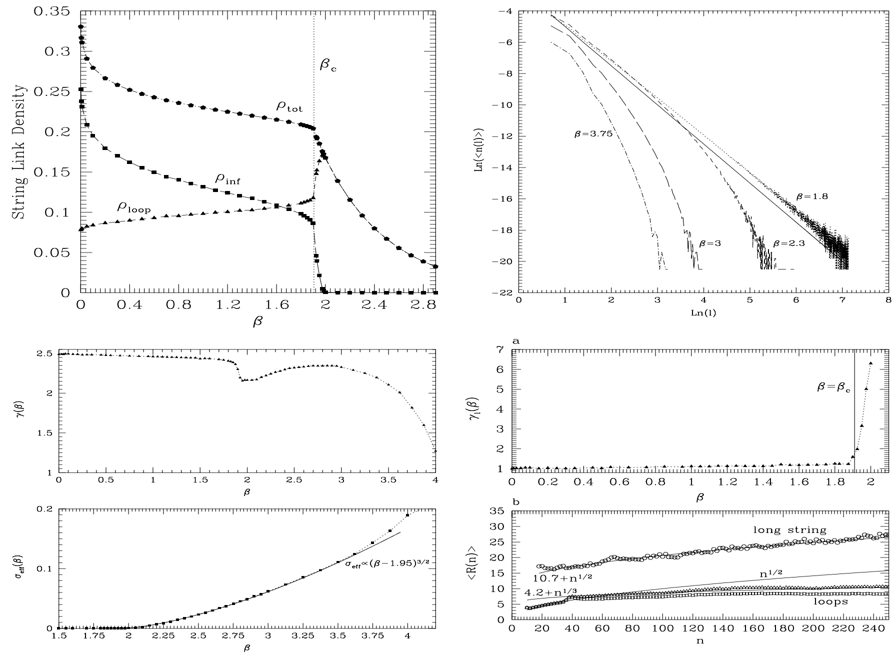

Figure 2: The phase transition in the 3D $O(2)$ model in terms of vortex strings. Fig. 1a (top left) shows how the string densities ρ change with T. In particular long strings $\rho_{\rm inf}$ appear at $T = T_c$. Fig. 1b shows the length distributions $n(l)$. At low T long strings are exponentially suppressed, but above T_c $n(l)$ becomes scale invariant, and approaches the Brownian case as $T \to \infty$. Fig. 1c shows how $\sigma_{\rm eff}$ and γ behave around T_c and Fig. 1d γ_l for long strings and $R(l)$, the distance between 2 points on the string *vs.* its length. This shows explicitly that short strings are self-seeking but long strings are essentially Brownian.

are self-seeking but long strings emerge as approximately Brownian. Similar results were obtained by Nguyen and Sudbo [18] and Kajantie *et al.* [19].

A related way of approaching the transition that is particularly useful in the statistical sampling of the partition function is to recognize, as in Figure 1, that as the critical point is approached typical configurations of the system are characterized by large domains over which the direction of the spin is aligned (except for small fluctuations). These clusters grow to percolate the volume at $T = T_c$ [15]. We see that in the boundaries between these large clusters strings can occur [short string loops can in principle also appear within the clusters]. Since the size of the clusters grows as the the critical point is approached so does the size of strings. At the critical point there will indeed be strings that percolate the volume, as we have seen directly above.

The description of the onset of criticality in terms of strings and in terms of (clusters of) spin is thus complementary. Clusters of spin are regions of local order delimited by local spin disorder, where macroscopic strings exist. Just as in the Ising case we can statistically describe the system in terms of these domains of order or equivalently in terms of their boundaries. Note however that the correspondence between strings and boundaries of phase is not an exact mapping (clearly there are phase boundaries where there are no strings), as was in the case of the Ising model.

There are universal quantities that must coincide as given by either description, as stressed recently by Schackel [16]. An example is the correlation length. Characteristic lengths can be associated of course with the size of typical strings or the size of correlated spin clusters. Although this size may not be exactly the same its associated critical exponent must coincide in the two pictures. The cluster distribution size $n_c(l)$ like the string length distribution is characterized by two quantities γ_c and $\sigma_c(T)$, where $\sigma_c \sim |T - T_c|^s$ in the critical region[c]. All field exponents can be related to γ_c and s, together with the dimensionality of space D, via scaling relations.

It is then suggestive that if strings are to give a correct description of the transition then their exponents may coincide with those of the cluster distribution [16]. With the current set of measurements [17,18,19] agreement of all exponents is not perfect: $\nu = s(\gamma_s - 1)/d$ works reasonably well, but other field exponents like α, γ, η require a larger value of γ_s, presently out of the range of current measurements, including their statistical uncertainties. The standing disagreement may be a result of the way vortex string distributions are constructed and measured or it may actually signal a failure of the string picture to yield a fully consistent description of the transition.

The preceding arguments work only under the condition that there is long range order that is gradually lost as the transition is approached from below. Once the disordered state is reached it becomes clear that long strings are possible at all temperatures, since over the volume all possible values of the phase is realized with equal probability. The size of the domains of different phases however remains a function of T. Again the size of these domains determines the characteristic length in the system - this length is closely related to distance between *long* strings. This has been confirmed by dynamical cooling of hot field configurations [20].

We close this section by recalling the analogy between the conductor-insulator transition that we explored in 2D. The analog in 3D of vortex pairs

[c]Below we refer to γ in (9) as γ_s to avoid confusion with the field exponent γ. s denotes the exponent of $\sigma_{\rm eff} \sim |T - T_c|^s$ for either strings or clusters.

are now short vortex loops. Long string, which appears as approximately free walks, corresponds to nucleating a loop of arbitrary length, in analogy to creating a pair of arbitrary separation in 2D. Indeed long string nucleation is first possible at $T = T_c$. This suggests that there is a "dual" microscopic model of the phase transition in terms of *interacting* walks: a line version of the Coulomb gas, with some appropriate potential, presumably that of the interaction between two static string segments. This picture has been explored in many instances [11], put it has been the accurate measurement of γ_c and s that permitted the construction of definite string models at criticality [21].

4 Conclusions and Outlook

In this lecture I explored the connection between topological excitations and critical phenomena in some $O(N)$ models.

As we have seen the understanding that second order transitions proceed by the occurrence of ever large correlated clusters, as T_c is approached from below, suggests the appearance of a scale invariant topological excitation population at T_c. The statistical distribution of defects in the critical domain must reflect that of phase domains and therefore is expected to be characterized by the same set of critical exponents. Then there will be a duality, valid in the critical domain, between the $O(N)$ partition function and that of an interacting ensemble of defects, at least for small N.

The question that remains is whether a statistical ensemble of defects alone can give the full picture of the transition. After all topological configurations do not describe all excitations. For example the low temperature phase of most $O(N)$ models is characterized by hydrodynamic modes, spin or sound waves. Can we make up these configurations in terms of vortices ? Clearly the answer is no, even if we used arbitrary vortex-antivortex configurations that carry no topological charge, there would be remaining short distance singularities sufficiently close to each of the defects.

Thus the thermodynamics of $O(N)$ models must differ in general, at least over small scales, from that of an ensemble of topological excitations. This difference may in some cases be irrelevant about the critical point. For example, it is conceivable that there is a system, written in terms of string degrees of freedom, that is in the same universality class as $O(2)$, but will differ by higher order irrelevant operators. After all vortices are not the whole description of the $O(2)$ model in 2D either, but they were the relevant degrees of freedom at criticality. Conversely, producing a model without strings but with the same critical exponents, would lead us to the conclusion that defects are unessential.

These issues now stand on a few well defined quantitative open questions, which will be decided theoretically in the near future. Concurrently, we may also hope that the topological excitation distribution exponents may be measured directly, see e.g. [4], by experiments seeking to study topological defect formation and evolution. Interesting new nonperturbative phenomenology may also result from the quantitative characterization of topological excitation behavior at high temperatures [22].

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